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Energy consumption maps for quaternary distillation sequences

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Abstract

Thermally coupled distillation columns represent a very interesting option for the intensification of distillation systems in order to reduce the energy consumption, and, as a consequence, the environmental impact of the separation process. Several thermally coupled distillation schemes can be generated for the separation of multicomponent mixtures. This fact is an advantage, since a wide portfolio of alternatives can be used to separate a specific mixture; however, this is also a disadvantage since a lot of alternatives must be explored in order to find the optimal one. The optimal configuration, for a given mixture, depends on the nature of the mixture, usually quantified for ternary mixtures through the ease of separation index (ESI), and also on the feed composition. As can be noticed, the size of the design and optimization problem increases when these variables are considered in the generation of the solutions space. For the separation of ternary mixtures, Tedder and Rudd (1978) presented a composition map for which thermally coupled systems allowed energy savings. However, the scenario is different for quaternary mixtures, since no similar information is available. Therefore, in this work, energy consumption data for five feed compositions for a mixture near to ideality are presented. The quaternary sequences studied are: conventional direct (three columns), conventional indirect (three columns), thermally coupled direct (main column and two side rectifiers), and thermally coupled indirect (main column and two side strippers). The design and optimization of the distillation sequences is performed through a multiobjective genetic algorithm with constraints handling, coupled to the commercial process simulator Aspen Plus, and enhanced through the use of neural networks.

Keywords: quaternary mixtures, energy consumption, thermally coupled distillation, stochastic optimization.

1. Introduction

It is well known that distillation is one of the most used separation processes for industrial mixtures. Its versatility relies on the fact that, with an adequate design, almost any purity can be reached. However, one of its main disadvantages is the elevated energy consumption, which is a consequence of a low thermodynamic efficiency. As the required purity increases, more energy must be provided to the column's reboiler. In order to maintain the advantages of distillation, and simultaneously reduce its energy requirements, several alternatives have been proposed. One of these options are the thermally coupled distillation columns, obtained substituting one or more auxiliary heat exchangers, associated to non product streams, with a vapour/liquid interconnecting stream. These systems avoid the phenomena known as re-mixing, taking advantage of the composition profiles (Triantafyllou and Smith, 1992); this allow decreasing the energy requirements and also the capital costs. There are several thermally coupled distillation schemes proposed for the separation of multicomponent mixtures. This fact is an advantage, since a wide set of alternatives can be used to separate a specific mixture; however, this is also a disadvantage since all the alternatives must be explored in order to identify the best one. The optimal sequence, for a given mixture, depends mainly on the nature of the mixture, usually quantified for ternary mixtures through the ease of separation index (ESI), and also on the feed composition. The ease of separation index was defined by Tedder and Rudd (1978), and it relates the distribution constant of each component of the mixture. As can be noticed, the size of the design and optimization problem increases when also these variables are considered in the generation of the solutions space. Some configurations have been proposed for the separation of quaternary mixtures, and it has been found that, for the cases reported, the use of quaternary thermally coupled distillation sequences may represent important reductions on energy consumptions showing also good control properties if compared to similar conventional sequences (Hernández et al., 2005, Errico et al., 2008, Vázquez-Castillo et al., 2009). Nevertheless, Shah and Agrawal (2010) evidenced that the use of thermal coupling could reduce the energy consumption only for some cases. This result is a generalization of the work of Tedder and Rudd (1978), where it was concluded that for ideal ternary mixtures, energy savings can be obtained by using thermally coupled sequences only if the composition of the middle-boiling component is between 0.4 and 0.8. Also in the same work, Tedder and Rudd presented composition maps for which thermally coupled systems allowed energy savings. In their study, eight distillation systems were analyzed for the separation of ternary mixtures, and energy consumption maps were generated as a function of the feed composition and nature of the mixture. This information was very useful, considering the large size of the solutions space when conventional and thermally coupled distillation columns are considered. However, the scenario is different for quaternary mixtures, since to the knowledge of the authors, there is no information about the composition space for which quaternary thermally coupled systems show lower energy requirements than conventional sequences. Therefore, in this work energy consumption data for five feed compositions for a mixture near to ideality are presented. The quaternary sequences studied are: conventional direct (three columns), conventional indirect (three columns), thermally coupled direct (main column and two side rectifiers), and thermally coupled indirect (main column and two side strippers). The set of compositions to be analyzed is obtained through an experimental design approach; in this work we are presenting a subset of 5 from the 11 resulting compositions. The optimal design of the distillation sequences is performed through a multiobjective genetic algorithm coupled to Aspen

Plus and speeded-up by the use of neural networks (Gutiérrez-Antonio and Briones-Ramírez, 2015).

2. Case of study

The mixture of 2-methyl-2-butene (A)/cyclopentane (B)/benzene (C)/toluene (D) has been taken as case of study. It can be seen that the mixture consists on ramified and cyclic hydrocarbons; thus, the Chao-Seader equation is used to model the vapour-liquid equilibrium. Feed flow rate for all cases is set as 100 kmol/h, with desired recoveries of 99% for all the components. The ease of separation index for this mixture, defined for the quaternary case as $ESI_{ABCD} = ESI_{ABC}/ESI_{BCD}$, is 1.04, which indicates ideality. In order to analyse the effect of feed composition on the energy requirements of the quaternary sequences, a set of values for feed compositions has been obtained through a simplex lattice experimental design approach. In this work, a sub-set of feed compositions is studied (Table 1). The configurations considered in the present study are reported in the Figure 1.

Table 1. Feed compositions used for the study.

Component/Case	**A**	**B**	**C**	**D**
M1F1	0.7	0.1	0.1	0.1
M1F2	0.1	0.7	0.1	0.1
M1F3	0.1	0.1	0.7	0.1
M1F4	0.1	0.1	0.1	0.7
M1F5	0.25	0.25	0.25	0.25

3. Design and optimization methodology

In order to generate the energy consumption data for the designs of conventional and thermally coupled quaternary sequences, a multiobjective genetic algorithm with constraints handling is used. We decided to employ this method since it has been proved to be a robust tool for the optimization of chemical processes. The genetic algorithm is coupled to the process simulator Aspen Plus; thus the complete rigorous model for distillation columns is used. A main problem with the use of the process simulator is the long time required to evaluate the objectives and constraints functions. Thus, the speed of the strategy is improved through the use of neuronal networks, which are used as surrogate models for the evaluation of the objectives and constraints functions. The code is implemented in Matlab, which is linked to Aspen Plus using ActiveX Technology. For more details the reader is referred to the original contribution (Gutiérrez-Antonio and Briones-Ramírez, 2015). For each system, a tuning process is performed to determine the number of generations and the number of individuals required. For the configurations analysed in this work, 1000 individuals are required per generation. The numbers of generations were 150 and 250 for conventional and thermally coupled distillation sequences, respectively. The main decision variables for the conventional configurations are the number of stages, the reflux ratio and location of feed stages. In the case of the thermally coupled sequences, the flow rates and locations of interlinking streams are also important design variables. The objective function involves the simultaneous minimization of the number of stages and heat duty for each sequence, while the constraints are the purities and recoveries established for all cases.

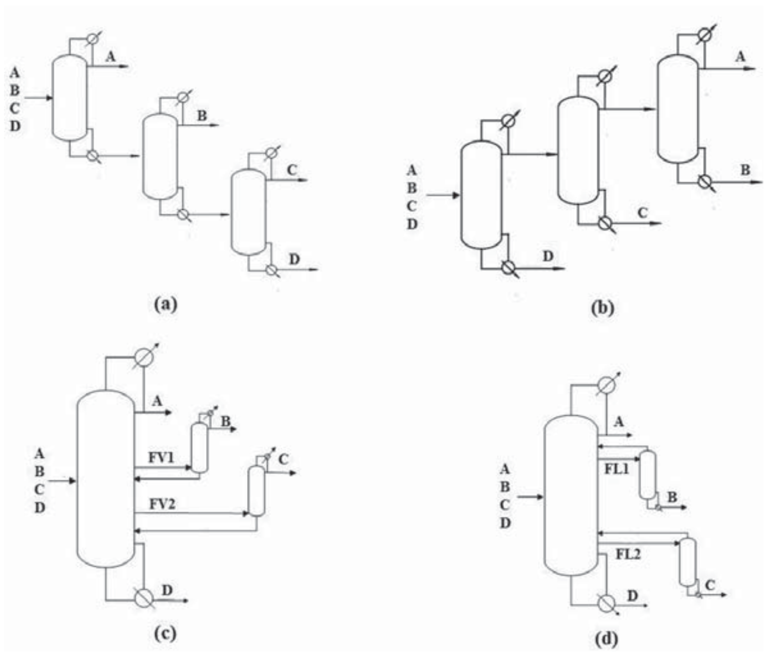

Figure 1. Studied distillation sequences: (a) Conventional direct sequence, CDS; (b) conventional indirect sequence, CIS; (c) quaternary thermally coupled direct sequence, QTCDS; (d) quaternary thermally coupled indirect sequence, QTCIS.

4. Results

In this section the results obtained in the optimization step are discussed in terms of energy consumption and number of stages; it is worth to mention that the objectives have been grouped in order to facilitate the presentation of the results. The Pareto front is integrated by a set of optimal designs including the minimum energy consumption, the minimum number of stages and all the designs in between these two extremes. Figure 2 shows the Pareto fronts for case M1F1, where objectives have been grouped.

From Figure 2, it is clear that for the same number of total stages, the minimum heat duty is observed in the QTCDS, whose optimal designs overlap in the region of less total stages with the CDS designs. The extremes of the Pareto front, which represent minimum energy requirements and minimum number of stages, respectively, are not of interest from the practical point of view. Considering this, some designs have been selected with a similar number of stages in order to observe changes in the heat duties. The Table 2 presents the heat duties of all analysed sequences for the five feed compositions, showed in Table 1, when 150 stages are considered. For the case M1F1, where component A is in major proportion, the best option for the separation of the four components is the QTCDS, followed by the CIS; for this feed composition it is clear that neither the QTCIS nor CDS are the optimal options to perform the separation.

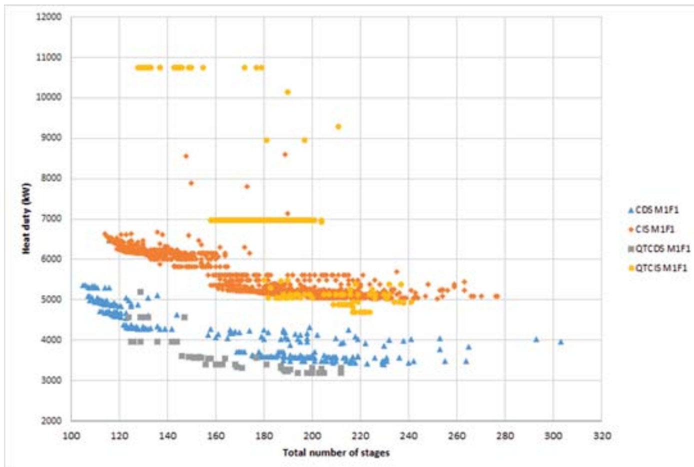

Figure 2. Pareto fronts of studied distillation sequences for case M1F1.

Table 2. Heat duties, Q_T, (kW) of all sequences for a similar number of total stages, N_T.

M1F1		
	N_T	Q_T
CDS	150	46,283.96
CIS	150	5,813.74
QTCDS	150	3,595.17
QTCIS	150	10,753.43

M1F2		
	N_T	Q_T
CDS	150	2,979.81
CIS	150	3,997.27
QTCDS	154	2,916.57
QTCIS	220	81,685.44

M1F3		
	N_T	Q_T
CDS	150	2,333.86
CIS	150	2,648.94
QTCDS	170	2,696.43
QTCIS	152	10,395.08

M1F4		
	N_T	Q_T
CDS	152	2,446.36
CIS	150	1,949.53
QTCDS	151	2,090.75
QTCIS	151	2,165.72

M1F5		
	N_T	Q_T
CDS	150	3,044.81
CIS	149	5,040.83
QTCDS	150	3,171.28
QTCIS	149	38,049.10

In the case M1F2, where component B is in major proportion, the best option for the separation of the four components is the QTCDS, followed by the CDS and the CIS; for this feed composition it is clear that the QTCIS is the worst option to perform the separation. On the other hand, the case M1F3, where component C is in major proportion, the best option for the separation is the CDS, followed by the CIS and the QTCDS; for this feed composition it is clear that the QTCIS is the worst option to perform the separation. For the case M1F4, where component D is in major proportion, the best option is the CDS, followed by the CIS and the QTCDS; for this feed composition it is clear that the QTCIS is the worst option to perform the separation. Finally, for case M1F5 the best option to perform the separation is the CDS, followed very close by the QTCDS; in this case the QTCIS is the worst option when a similar number of stages is considered.

5. Conclusions

In this work, an analysis of the effect of feed composition on the energy requirements of quaternary thermally coupled distillation sequences has been presented. A stochastic optimization methodology has been used for the design of the distillation sequences. It has been found that, for a mixture close to ideality, the quaternary thermally coupled distillation sequences show energy savings only for a mixture with high feed composition of the light components. The conventional indirect sequence is preferred when the heavy component has high composition, because it is separated in the first column. For an equimolar mixture, the direct conventional sequence is the best alternative, but the difference with the thermally coupled distillation sequence is small. When the third component has the highest feed composition, the conventional direct sequence must be preferred. Nevertheless, further studies are required to analyse a wider range of compositions.

References

M. Errico, B.-G. Rong, G. Tola, I. Turunen, 2008, Process intensification for the retrofit of a multicomponent distillation plant – an industrial case study, Ind. Eng. Chem. Res., 47, 1975-1980

C. Gutiérrez-Antonio, A. Briones-Ramírez, 2015, Multiobjective Stochastic Optimization of Dividing-wall Distillation Columns Using a Surrogate Model Based on Neural Networks, Chem. and Biochem. Eng. Quat., 29(4), 491-504

S. Hernández, I.R. Gudiño-Mares, J.C. Cárdenas, J.G. Segovia-Hernández, V. Rico-Ramírez, 2005, Analysis of control properties of thermally coupled distillation sequences for four-component mixtures, Ind. Eng. Chem. Res., 44, Issue 2, 391-399

V.H. Shah, R. Agrawal, 2011, Are all thermal coupling links between multicomponent distillation columns useful from an energy perspective?, Ind. Eng. Chem. Res., 50, Issue 3, 1770-1777

D.W. Tedder, D.F. Rudd, 1978, Parametric studies in industrial distillation: Part I. Design comparisons, AIChE J., 24, Issue 2, 303-315

C. Triantafyllou, R. Smith, 1992, The design and optimization of fully thermally coupled distillation, Trans. Inst. Chem. Eng., 70, Part A, 118-132

J.A. Vázquez-Castillo, J.A. Venegas-Sánchez, J.G. Segovia-Hernández, H. Hernández-Escoto, S. Hernández, C. Gutiérrez-Antonio, A. Briones-Ramírez, 2009, Design and optimization, using genetic algorithms, of intensified distillation systems for a class of quaternary mixtures, Comput. Chem. Eng., 33, Issue 11, 1841-1850